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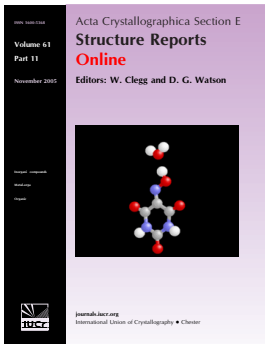

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Dicyclohexylammonium trimethylbis(hydrogen phenylphosphonato)stannate(IV)

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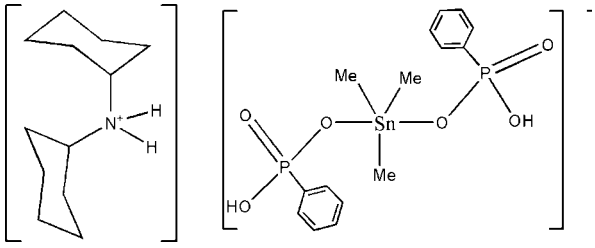
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.007 Å; R factor = 0.047; wR factor = 0.124; data-to-parameter ratio = 20.4.

In the title compound, $(C_{12}H_{24}N)[Sn(CH_3)_3(C_6H_6O_3P)_2]$, the $SnMe_3$ residues are axially coordinated by two monodentate $[PhPO_3H]^-$ anions, leading to a trigonal–bipyramidal geometry for the Sn^{IV} atom. The two $[SnMe_3(PhPO_3H)_2]^-$ anions in the unit cell are associated into infinite chains along the *a* axis by O—H···O hydrogen bonds involving the hydroxy group of the hydrogen phenylphosphonate ion. The chains interact with one another *via* O—H···O hydrogen bonds along the *c* axis. These networks of anions assemble with the dicyclohexylammonium ion through N—H···O hydrogen bonds, forming a three-dimensional network.

Related literature

For related organotin derivatives, see: Weakley (1976); Molloy *et al.* (1981); Evans & Karpel (1985); Gielen *et al.* (1995); Yin & Wang (2004); Kapoor *et al.* (2005); Zhang *et al.* (2006). For our recent work on the coordination ability of oxyanions, see: Diop *et al.* (2002, 2003); Diallo *et al.* (2009).



Experimental

Crystal data

$(C_{12}H_{24}N)[Sn(CH_3)_3(C_6H_6O_3P)_2]$
M_r = 660.27
Triclinic, $P\overline{1}$
a = 10.8718 (5) Å
b = 12.7103 (7) Å
c = 13.3218 (7) Å
α = 100.625 (3)°
β = 103.687 (3)°
γ = 111.996 (3)°
V = 1580.41 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.95 mm^{-1}
T = 150 K
0.45 × 0.30 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.675, T_{max} = 0.833
21070 measured reflections
7212 independent reflections
6014 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.124
S = 1.09
7212 reflections
353 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.86 e Å^{-3}
$\Delta\rho_{min}$ = −1.80 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn—C1	2.132 (4)	Sn—O1	2.227 (2)
Sn—C2	2.114 (4)	Sn—O4	2.241 (3)
Sn—C3	2.134 (4)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O6^{i}	0.76 (4)	1.88 (4)	2.642 (4)	178 (7)
O5—H5A···O6^{ii}	0.94 (7)	1.67 (7)	2.596 (4)	169 (6)
N—H10A···O3	0.89 (2)	1.92 (2)	2.798 (4)	169 (4)
N—H10B···O3^{iii}	0.95 (4)	1.83 (4)	2.759 (4)	165 (4)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+1, -z+1$; (iii) $-x+2, -y+2, -z+1$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VN2021).

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supplementary materialsm

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Dicyclohexylammonium trimethylbis(hydrogen phenylphosphonato)stannate(IV)t

T. Diop, L. Diop, C. A. K. Diop, K. C. Molloy and G. Kociok-Köhnt

Comment

Research on organotin derivatives has been an attractive area because of their numerous applications and their versatilev structure (Evans & Karpel, 1985; Kapoor *et al.*, 2005; Zhang *et al.*, 2006; Yin & Wang, 2004; Gielen *et al.*, 1995). In thev scope of our research work on the coordination ability of oxyanions (Diop *et al.*, 2002, Diallo *et al.*, 2009; Diop *et al.*,v 2003) and our interest to synthesize new organotin derivatives for biological tests, we elucidate here the structure of the titlev compound, [$C_{15}H_{21}O_6P_2Sn$,$C_{12}H_{24}N$] (Fig. 1).v

The crystal structure of the molecule is shown in Fig 2: hydrogen bonds between pairs of $[SnMe_3(PhPO_3H)_2]^-$ generatev a six membered ring, comprise a honey comb network by virtue of the hydrogen bonds between the ligands as in *catena*-v trimethyltin(IV)phenylarsenate, reported by Diop *et al. (*2002).v

Each $SnMe_3$ unit is σ bonded to two $[PhPO_3H]^-$ via one negatively charged oxygen atom, leading to a *trans* tri-v gonal bipyramidal environment around the tin centre (Fig. 1). The resulting anions $[SnMe_3(PhPO_3H)_2]^-$ are associatedv through hydrogen bonds OH···O, along the *b* axis into pairs and along the *a* axis to form infinite layers (Fig. 2). Thev different layers are connected by NH···O hydrogen bonds along the *b* axis. The hydrogen bonds render the P=O andv P—O bond distances almost egal (P(1)—O(3)1.506 (3) Å, P(1)—O(1): 1.509 (2) Å, P(1)—O(2): 1.569 (3) Å) whilev different of those in the parent phenylphosphonic acid $PhPO_3H_2$ (Weakley, 1976) (1.496 Å for P=O and 1.545 Åv for P—OH). The geometry around the phosphorous atom in the ligands is a distorted tetrahedron (O(3)—P(1)—O(1):v 115.48°(15), O(1)—P(1)—C(4): 107.03°(15)) owing to steric hindrance. The sum of the C—Sn—C angle is 59.99° andv the O(1)—Sn—O(4) angle of 178.24°(9) indicate a nearly perfect *trans* trigonal bipyramidal arrangement with the carbonv atoms of the methyl occupying the equatorial positions while the oxygen atoms are on the apical positions. The two Sn—Ov distances observed here - Sn—O(1) 2.227 (2) Å; Sn—O(4) 2.240 (3) Å - are shorter than the distances reported for(α-v phenylphosphonato)trimethyltin(IV) by Molloy *et al.* (1981) (2.240 (6) Å and 2.319 (5) Å).v

Experimental

$Cy_2NH_2PhPO_3H$ (*L*) is obtained on mixing dicyclohexylamine with $PhPO_3H_2$ in water in 1/1 ratio. The title compoundv has been obtained as white crystalline solid by reacting (*L*) with trimetyltinchloride in ethanol (2/1 ratio *M.* p:170°). Slowv solvent evaporation of the solution afforded colorless crystals suitable for x-ray structure determination. All the chemicalsv (Aldrich) were used without any further purification.v

Refinement

All C-bound H-atoms were positioned geometrically and were included in the refinement in the riding model approximation,v with Uĩso~(H) set to 1.2 and 1.5 U~eq~(C). All N- and O-bound H-atoms have been located in the difference Fourier mapv

and were refined freely. However, H(2) binding to O(2) and H(10A) binding to N had to be restrained with O—H = 0.82 (2)v Å and N—H = 0.87 (2) Å.v

Figures

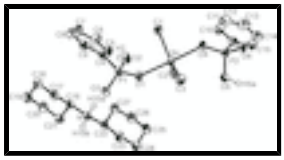

Fig. 1. : The molecular structure of the title compound with the atom-numbering scheme. Dis-v placement ellipsoids are drawn at the 50% probability level.v

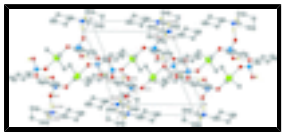

Fig. 2. : Three dimensional structure showing the hydrogen bonds as dotted lines.v

Dicyclohexylammonium bis(hydrogen phenylphosphonato)trimethylstannate(IV)

Crystal data

$(C_{12}H_{24}N)[Sn(CH_3)_3(C_6H_6O_3P)_2]$v	Z = 2v
M_r = 660.27v	$F(000)$ = 684v
Triclinic, $P\overline{1}$v	D_x = 1.387 Mg m^{-3}v
Hall symbol: -P 1v	Mo $K\alpha$ radiation, λ = 0.71073 Åv
a = 10.8718 (5) Åv	Cell parameters from 47204 reflectionsv
b = 12.7103 (7) Åv	θ = 2.9–27.5°v
c = 13.3218 (7) Åv	μ = 0.95 mm^{-1}v
α = 100.625 (3)°v	T = 150 Kv
β = 103.687 (3)°v	Plate, colourlessv
γ = 111.996 (3)°v	0.45 × 0.30 × 0.20 mmv
V = 1580.41 (14) Å^{3}v	

Data collection

Nonius KappaCCDv diffractometerv	7212 independent reflectionsv
Radiation source: fine-focus sealed tubev	6014 reflections with $I > 2\sigma(I)$v
graphitev	$_{int}$ = 0.068v
166 2.0 degree images with ω scansv	θ_{max} = 27.5°, θ_{min} = 3.8°v
Absorption correction: multi-scanv (*SORTAV*; Blessing, 1995)v	h = −14→14v
T_{min} = 0.675, T_{max} = 0.833v	k = −16→16v
21070 measured reflectionsv	l = −17→16

Refinement

Refinement on F^2v	Primary atom site location: structure-invariant directv methodsv
Least-squares matrix: fullv	Secondary atom site location: difference Fourier mapv

$[F^2 > 2\sigma(F^2)] = 0.047$v	Hydrogen site location: inferred from neighbouringv sitesv
$wR(F^2) = 0.124$v	H atoms treated by a mixture of independent and constrained refinementv
$S = 1.09$v	$w = 1/[\sigma^2(F_o^2) + (0.0655P)^2 + 1.1841P]$ where $P = (F_o^2 + 2F_c^2)/3$v
7212 reflectionsv	$(\Delta/\sigma)_{max} < 0.001$v
353 parametersv	$\Delta\rho_{max} = 1.86$ e Å^{-3}v
2 restraintsv	$\Delta\rho_{min} = -1.80$ e Å^{-3}v

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance mat-v rix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlationsv between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment ofv cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.v

Refinement. Refinement of F^2 against ALL reflections. The weighted v-factor *wR* and goodness of fit *S* are based on F^2, convention-v al v-factors v are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating v-v factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. v-factors based on F^2 are statistically about twice as largev as those based on *F*, and v- factors based on ALL data will be even larger.v

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}v
Snv	0.39323 (2)v	0.58948 (2)v	0.341865 (19)v	0.02776 (9)v
P1v	0.74338 (9)v	0.72317 (8)v	0.37030 (7)v	0.02711 (19)v
P2v	0.06261 (9)v	0.44906 (8)v	0.36638 (8)v	0.02827 (19)v
O1v	0.6010 (2)v	0.7236 (2)v	0.3496 (2)v	0.0320 (5)v
O2v	0.7419 (3)v	0.6228 (2)v	0.4238 (2)v	0.0353 (6)v
H2v	0.807 (5)v	0.623 (5)v	0.462 (4)v	0.070 (18)*v
O3v	0.8675 (2)v	0.8403 (2)v	0.4370 (2)v	0.0310 (5)v
O4v	0.1834 (3)v	0.4514 (2)v	0.3290 (2)v	0.0360 (6)v
O5v	0.0892 (3)v	0.5817 (2)v	0.4150 (2)v	0.0338 (6)v
H5Av	0.039 (7)v	0.585 (6)v	0.463 (5)v	0.08 (2)*v
O6v	0.0351 (2)v	0.3812 (2)v	0.4473 (2)v	0.0306 (5)v
Nv	0.9314 (3)v	1.0380 (3)v	0.3600 (2)v	0.0291 (6)v
H10Av	0.906 (5)v	0.970 (3)v	0.376 (4)v	0.043 (12)*v
H10Bv	1.004 (4)v	1.092 (4)v	0.426 (3)v	0.029 (10)*v
C1v	0.4197 (4)v	0.4478 (4)v	0.2508 (3)v	0.0357 (8)v
H1Av	0.3304v	0.3754v	0.2223v	0.053*v
H1Bv	0.4921v	0.4334v	0.2977v	0.053*v
H1Cv	0.4488v	0.4694v	0.1904v	0.053*v
C2v	0.4641 (4)v	0.6421 (4)v	0.5132 (3)v	0.0373 (8)v
H2Av	0.5502v	0.6326v	0.5399v	0.056*v
H2Bv	0.3912v	0.5924v	0.5378v	0.056*v
H2Cv	0.4837v	0.7257v	0.5412v	0.056*v
C3v	0.2929 (4)v	0.6733 (4)v	0.2497 (3)v	0.0396 (9)v

H3Av	0.2375v	0.6994v	0.2876v	0.059*v
H3Bv	0.2307v	0.6166v	0.1782v	0.059*v
H3Cv	0.3646v	0.7424v	0.2409v	0.059*v
C4v	0.7614 (4)v	0.6798 (3)v	0.2399 (3)v	0.0297 (7)v
C5v	0.6643 (4)v	0.6721 (4)v	0.1461 (3)v	0.0433 (10)v
H5v	0.5856v	0.6861v	0.1506v	0.052*v
C6v	0.6811 (6)v	0.6443 (6)v	0.0462 (4)v	0.0610 (14)v
H6v	0.6148v	0.6405v	−0.0170v	0.073*v
C7v	0.7947 (5)v	0.6219 (5)v	0.0383 (3)v	0.0516 (11)v
H7v	0.8058v	0.6026v	−0.0304v	0.062*v
C8v	0.8919 (5)v	0.6278 (4)v	0.1304 (4)v	0.0430 (9)v
H8v	0.9689v	0.6115v	0.1252v	0.052*v
C9v	0.8754 (4)v	0.6579 (3)v	0.2309 (3)v	0.0355 (8)v
H9v	0.9430v	0.6635v	0.2942v	0.043*v
C10v	−0.0932 (4)v	0.3826 (3)v	0.2475 (3)v	0.0322 (7)v
C11v	−0.0850 (5)v	0.3461 (4)v	0.1446 (3)v	0.0444 (10)v
H11v	0.0032v	0.3562v	0.1372v	0.053*v
C12v	−0.2058 (6)v	0.2946 (5)v	0.0527 (4)v	0.0562 (12)v
H12v	−0.2001v	0.2691v	−0.0170v	0.067*v
C13v	−0.3337 (6)v	0.2812 (5)v	0.0639 (4)v	0.0595 (13)v
H13v	−0.4159v	0.2462v	0.0014v	0.071*v
C14v	−0.3430 (5)v	0.3180 (4)v	0.1645 (4)v	0.0512 (11)v
H14v	−0.4314v	0.3085v	0.1711v	0.061*v
C15v	−0.2241 (4)v	0.3688 (4)v	0.2559 (3)v	0.0391 (9)v
H15v	−0.2312v	0.3946v	0.3250v	0.047*v
C16v	0.9824 (4)v	1.0236 (3)v	0.2651 (3)v	0.0314 (7)v
H16v	0.9017v	0.9615v	0.2010v	0.038*v
C17v	1.0365 (5)v	1.1398 (4)v	0.2371 (3)v	0.0406 (9)v
H17Av	1.1137v	1.2033v	0.3008v	0.049*v
H17Bv	0.9597v	1.1641v	0.2179v	0.049*v
C18v	1.0900 (5)v	1.1238 (4)v	0.1419 (4)v	0.0465 (10)v
H18Av	1.1312v	1.2012v	0.1279v	0.056*v
H18Bv	1.0099v	1.0674v	0.0761v	0.056*v
C19v	1.2011 (5)v	1.0767 (4)v	0.1639 (4)v	0.0470 (10)v
H19Av	1.2276v	1.0617v	0.0984v	0.056*v
H19Bv	1.2864v	1.1377v	0.2237v	0.056*v
C20v	1.1468 (4)v	0.9626 (4)v	0.1941 (4)v	0.0438 (9)v
H20Av	1.2227v	0.9371v	0.2122v	0.053*v
H20Bv	1.0678v	0.8990v	0.1315v	0.053*v
C21v	1.0967 (4)v	0.9810 (4)v	0.2915 (3)v	0.0376 (8)v
H21Av	1.0590v	0.9053v	0.3089v	0.045*v
H21Bv	1.1770v	1.0408v	0.3557v	0.045*v
C22v	0.8128 (4)v	1.0751 (3)v	0.3484 (3)v	0.0325 (8)v
H22v	0.8446v	1.1542v	0.3349v	0.039*v
C23v	0.7833 (4)v	1.0885 (4)v	0.4551 (3)v	0.0395 (9)v
H23Av	0.7567v	1.0119v	0.4717v	0.047*v
H23Bv	0.8695v	1.1491v	0.5144v	0.047*v
C24v	0.6648 (4)v	1.1259 (4)v	0.4481 (4)v	0.0472 (10)v
H24Av	0.6941v	1.2052v	0.4367v	0.057*v

H24Bv	0.6447v	1.1319v	0.5171v	0.057*v
C25v	0.5317 (4)v	1.0355 (4)v	0.3547 (4)v	0.0499 (11)v
H25Av	0.4982v	0.9577v	0.3690v	0.060*v
H25Bv	0.4568v	1.0626v	0.3497v	0.060*v
C26v	0.5605 (4)v	1.0211 (4)v	0.2482 (4)v	0.0493 (11)v
H26Av	0.5843v	1.0969v	0.2302v	0.059*v
H26Bv	0.4745v	0.9591v	0.1897v	0.059*v
C27v	0.6824 (4)v	0.9860 (4)v	0.2541 (3)v	0.0377 (8)v
H27Av	0.6544v	0.9057v	0.2632v	0.045*v
H27Bv	0.7035v	0.9833v	0.1856v	0.045*v

Atomic displacement parameters (Å^2)

	U^{11v}	U^{22v}	U^{33v}	U^{12v}	U^{13v}	U^{23v}
Snv	0.02108 (13)v	0.03255 (14)v	0.03159 (14)v	0.01278 (10)v	0.00933 (9)v	0.01115 (9)v
P1v	0.0195 (4)v	0.0280 (4)v	0.0322 (4)v	0.0092 (4)v	0.0066 (3)v	0.0106 (3)v
P2v	0.0206 (4)v	0.0297 (5)v	0.0366 (5)v	0.0116 (4)v	0.0107 (3)v	0.0121 (4)v
O1v	0.0219 (12)v	0.0349 (13)v	0.0415 (14)v	0.0131 (11)v	0.0104 (10)v	0.0156 (11)v
O2v	0.0234 (13)v	0.0372 (14)v	0.0439 (15)v	0.0105 (11)v	0.0067 (11)v	0.0213 (12)v
O3v	0.0209 (11)v	0.0320 (13)v	0.0333 (13)v	0.0073 (10)v	0.0059 (9)v	0.0086 (10)v
O4v	0.0254 (12)v	0.0364 (14)v	0.0504 (16)v	0.0141 (11)v	0.0181 (11)v	0.0146 (12)v
O5v	0.0296 (13)v	0.0310 (13)v	0.0426 (14)v	0.0128 (11)v	0.0144 (11)v	0.0134 (11)v
O6v	0.0243 (12)v	0.0317 (13)v	0.0379 (13)v	0.0132 (11)v	0.0100 (10)v	0.0138 (10)v
Nv	0.0240 (14)v	0.0287 (16)v	0.0314 (15)v	0.0098 (13)v	0.0065 (12)v	0.0097 (12)v
C1v	0.0299 (18)v	0.041 (2)v	0.039 (2)v	0.0182 (17)v	0.0129 (15)v	0.0108 (16)v
C2v	0.038 (2)v	0.045 (2)v	0.038 (2)v	0.0237 (18)v	0.0148 (16)v	0.0166 (17)v
C3v	0.0293 (18)v	0.045 (2)v	0.048 (2)v	0.0175 (17)v	0.0108 (16)v	0.0216 (18)v
C4v	0.0246 (16)v	0.0316 (18)v	0.0337 (18)v	0.0129 (15)v	0.0089 (13)v	0.0116 (14)v
C5v	0.034 (2)v	0.061 (3)v	0.037 (2)v	0.028 (2)v	0.0082 (16)v	0.0097 (18)v
C6v	0.054 (3)v	0.100 (4)v	0.036 (2)v	0.048 (3)v	0.008 (2)v	0.013 (2)v
C7v	0.057 (3)v	0.074 (3)v	0.034 (2)v	0.036 (3)v	0.0198 (19)v	0.014 (2)v
C8v	0.042 (2)v	0.049 (2)v	0.049 (2)v	0.029 (2)v	0.0184 (18)v	0.0150 (19)v
C9v	0.0273 (18)v	0.039 (2)v	0.041 (2)v	0.0154 (16)v	0.0094 (15)v	0.0140 (16)v
C10v	0.0314 (18)v	0.0330 (19)v	0.0383 (19)v	0.0183 (16)v	0.0124 (15)v	0.0146 (15)v
C11v	0.047 (2)v	0.054 (3)v	0.042 (2)v	0.029 (2)v	0.0163 (18)v	0.0181 (19)v
C12v	0.064 (3)v	0.067 (3)v	0.039 (2)v	0.037 (3)v	0.009 (2)v	0.014 (2)v
C13v	0.053 (3)v	0.059 (3)v	0.050 (3)v	0.030 (3)v	−0.009 (2)v	0.005 (2)v
C14v	0.031 (2)v	0.051 (3)v	0.063 (3)v	0.021 (2)v	0.0031 (19)v	0.009 (2)v
C15v	0.0289 (18)v	0.042 (2)v	0.045 (2)v	0.0182 (17)v	0.0095 (16)v	0.0103 (17)v
C16v	0.0270 (17)v	0.0316 (18)v	0.0313 (17)v	0.0097 (15)v	0.0087 (14)v	0.0080 (14)v
C17v	0.047 (2)v	0.036 (2)v	0.044 (2)v	0.0195 (19)v	0.0187 (18)v	0.0167 (17)v
C18v	0.055 (3)v	0.046 (2)v	0.044 (2)v	0.021 (2)v	0.025 (2)v	0.0191 (19)v
C19v	0.039 (2)v	0.052 (3)v	0.049 (2)v	0.016 (2)v	0.0211 (19)v	0.015 (2)v
C20v	0.035 (2)v	0.046 (2)v	0.050 (2)v	0.0188 (19)v	0.0157 (18)v	0.0097 (19)v
C21v	0.0325 (19)v	0.038 (2)v	0.043 (2)v	0.0164 (17)v	0.0136 (16)v	0.0127 (16)v
C22v	0.0248 (17)v	0.0293 (18)v	0.042 (2)v	0.0122 (15)v	0.0079 (14)v	0.0116 (15)v
C23v	0.0301 (19)v	0.044 (2)v	0.042 (2)v	0.0158 (17)v	0.0132 (16)v	0.0075 (17)v
C24v	0.033 (2)v	0.047 (2)v	0.058 (3)v	0.0178 (19)v	0.0167 (19)v	0.006 (2)v

C25v	0.0269 (19)v	0.044 (2)v	0.071 (3)v	0.0136 (18)v	0.0155 (19)v	0.005 (2)v
C26v	0.029 (2)v	0.049 (3)v	0.058 (3)v	0.0165 (19)v	0.0013 (18)v	0.008 (2)v
C27v	0.0280 (18)v	0.041 (2)v	0.040 (2)v	0.0156 (17)v	0.0054 (15)v	0.0096 (16)v

Geometric parameters (Å, °)

Sn—C1v	2.132 (4)v	C11—H11v	0.9500v
Sn—C2v	2.114 (4)v	C12—C13v	1.383 (8)v
Sn—C3v	2.134 (4)v	C12—H12v	0.9500v
Sn—O1v	2.227 (2)v	C13—C14v	1.376 (7)v
Sn—O4v	2.241 (3)v	C13—H13v	0.9500v
P1—O3v	1.506 (3)v	C14—C15v	1.383 (6)v
P1—O1v	1.509 (2)v	C14—H14v	0.9500v
P1—O2v	1.569 (3)v	C15—H15v	0.9500v
P1—C4v	1.803 (4)v	C16—C17v	1.524 (5)v
P2—O4v	1.503 (3)v	C16—C21v	1.525 (5)v
P2—O6v	1.516 (3)v	C16—H16v	1.0000v
P2—O5v	1.578 (3)v	C17—C18v	1.527 (6)v
P2—C10v	1.805 (4)v	C17—H17Av	0.9900v
O2—H2v	0.76 (4)v	C17—H17Bv	0.9900v
O5—H5Av	0.94 (7)v	C18—C19v	1.529 (6)v
N—C16v	1.503 (5)v	C18—H18Av	0.9900v
N—C22v	1.515 (5)v	C18—H18Bv	0.9900v
N—H10Av	0.887 (19)v	C19—C20v	1.517 (6)v
N—H10Bv	0.95 (4)v	C19—H19Av	0.9900v
C1—H1Av	0.9800v	C19—H19Bv	0.9900v
C1—H1Bv	0.9800v	C20—C21v	1.534 (6)v
C1—H1Cv	0.9800v	C20—H20Av	0.9900v
C2—H2Av	0.9800v	C20—H20Bv	0.9900v
C2—H2Bv	0.9800v	C21—H21Av	0.9900v
C2—H2Cv	0.9800v	C21—H21Bv	0.9900v
C3—H3Av	0.9800v	C22—C27v	1.517 (5)v
C3—H3Bv	0.9800v	C22—C23v	1.522 (5)v
C3—H3Cv	0.9800v	C22—H22v	1.0000v
C4—C5v	1.393 (5)v	C23—C24v	1.521 (5)v
C4—C9v	1.395 (5)v	C23—H23Av	0.9900v
C5—C6v	1.385 (6)v	C23—H23Bv	0.9900v
C5—H5v	0.9500v	C24—C25v	1.528 (6)v
C6—C7v	1.390 (7)v	C24—H24Av	0.9900v
C6—H6v	0.9500v	C24—H24Bv	0.9900v
C7—C8v	1.386 (6)v	C25—C26v	1.517 (7)v
C7—H7v	0.9500v	C25—H25Av	0.9900v
C8—C9v	1.395 (6)v	C25—H25Bv	0.9900v
C8—H8v	0.9500v	C26—C27v	1.539 (6)v
C9—H9v	0.9500v	C26—H26Av	0.9900v
C10—C11v	1.399 (5)v	C26—H26Bv	0.9900v
C10—C15v	1.401 (5)v	C27—H27Av	0.9900v
C11—C12v	1.398 (6)v	C27—H27Bv	0.9900v
C2—Sn—C1v	121.15 (15)v	C12—C13—H13v	119.7v

C2—Sn—C3v	122.89 (16)v	C13—C14—C15v	120.1 (4)v
C1—Sn—C3v	115.97 (16)v	C13—C14—H14v	119.9v
C2—Sn—O1v	88.92 (13)v	C15—C14—H14v	119.9v
C1—Sn—O1v	91.77 (12)v	C14—C15—C10v	120.6 (4)v
C3—Sn—O1v	89.14 (13)v	C14—C15—H15v	119.7v
C2—Sn—O4v	92.68 (13)v	C10—C15—H15v	119.7v
C1—Sn—O4v	86.78 (13)v	N—C16—C17v	110.9 (3)v
C3—Sn—O4v	90.59 (13)v	N—C16—C21v	109.1 (3)v
O1—Sn—O4v	178.24 (9)v	C17—C16—C21v	111.2 (3)v
O3—P1—O1v	115.48 (15)v	N—C16—H16v	108.5v
O3—P1—O2v	110.97 (15)v	C17—C16—H16v	108.5v
O1—P1—O2v	107.81 (15)v	C21—C16—H16v	108.5v
O3—P1—C4v	108.23 (15)v	C16—C17—C18v	110.1 (3)v
O1—P1—C4v	107.03 (15)v	C16—C17—H17Av	109.6v
O2—P1—C4v	106.94 (16)v	C18—C17—H17Av	109.6v
O4—P2—O6v	115.57 (15)v	C16—C17—H17Bv	109.6v
O4—P2—O5v	108.23 (15)v	C18—C17—H17Bv	109.6v
O6—P2—O5v	110.03 (15)v	H17A—C17—H17Bv	108.2v
O4—P2—C10v	107.22 (17)v	C17—C18—C19v	111.8 (4)v
O6—P2—C10v	108.73 (16)v	C17—C18—H18Av	109.3v
O5—P2—C10v	106.67 (16)v	C19—C18—H18Av	109.3v
P1—O1—Snv	132.28 (15)v	C17—C18—H18Bv	109.3v
P1—O2—H2v	125 (5)v	C19—C18—H18Bv	109.3v
P2—O4—Snv	136.69 (16)v	H18A—C18—H18Bv	107.9v
P2—O5—H5Av	110 (4)v	C20—C19—C18v	111.4 (4)v
C16—N—C22v	117.5 (3)v	C20—C19—H19Av	109.3v
C16—N—H10Av	107 (3)v	C18—C19—H19Av	109.3v
C22—N—H10Av	109 (3)v	C20—C19—H19Bv	109.3v
C16—N—H10Bv	114 (2)v	C18—C19—H19Bv	109.3v
C22—N—H10Bv	106 (2)v	H19A—C19—H19Bv	108.0v
H10A—N—H10Bv	102 (4)v	C19—C20—C21v	110.7 (3)v
Sn—C1—H1Av	109.5v	C19—C20—H20Av	109.5v
Sn—C1—H1Bv	109.5v	C21—C20—H20Av	109.5v
H1A—C1—H1Bv	109.5v	C19—C20—H20Bv	109.5v
Sn—C1—H1Cv	109.5v	C21—C20—H20Bv	109.5v
H1A—C1—H1Cv	109.5v	H20A—C20—H20Bv	108.1v
H1B—C1—H1Cv	109.5v	C16—C21—C20v	109.7 (3)v
Sn—C2—H2Av	109.5v	C16—C21—H21Av	109.7v
Sn—C2—H2Bv	109.5v	C20—C21—H21Av	109.7v
H2A—C2—H2Bv	109.5v	C16—C21—H21Bv	109.7v
Sn—C2—H2Cv	109.5v	C20—C21—H21Bv	109.7v
H2A—C2—H2Cv	109.5v	H21A—C21—H21Bv	108.2v
H2B—C2—H2Cv	109.5v	N—C22—C27v	111.3 (3)v
Sn—C3—H3Av	109.5v	N—C22—C23v	108.1 (3)v
Sn—C3—H3Bv	109.5v	C27—C22—C23v	111.6 (3)v
H3A—C3—H3Bv	109.5v	N—C22—H22v	108.6v
Sn—C3—H3Cv	109.5v	C27—C22—H22v	108.6v
H3A—C3—H3Cv	109.5v	C23—C22—H22v	108.6v
H3B—C3—H3Cv	109.5v	C24—C23—C22v	110.4 (3)v

C5—C4—C9v	118.5 (3)v	C24—C23—H23Av	109.6v
C5—C4—P1v	120.5 (3)v	C22—C23—H23Av	109.6v
C9—C4—P1v	121.0 (3)v	C24—C23—H23Bv	109.6v
C6—C5—C4v	120.8 (4)v	C22—C23—H23Bv	109.6v
C6—C5—H5v	119.6v	H23A—C23—H23Bv	108.1v
C4—C5—H5v	119.6v	C23—C24—C25v	110.5 (4)v
C5—C6—C7v	120.1 (4)v	C23—C24—H24Av	109.5v
C5—C6—H6v	119.9v	C25—C24—H24Av	109.5v
C7—C6—H6v	119.9v	C23—C24—H24Bv	109.5v
C8—C7—C6v	120.1 (4)v	C25—C24—H24Bv	109.5v
C8—C7—H7v	120.0v	H24A—C24—H24Bv	108.1v
C6—C7—H7v	120.0v	C26—C25—C24v	110.8 (4)v
C7—C8—C9v	119.4 (4)v	C26—C25—H25Av	109.5v
C7—C8—H8v	120.3v	C24—C25—H25Av	109.5v
C9—C8—H8v	120.3v	C26—C25—H25Bv	109.5v
C8—C9—C4v	121.1 (4)v	C24—C25—H25Bv	109.5v
C8—C9—H9v	119.4v	H25A—C25—H25Bv	108.1v
C4—C9—H9v	119.4v	C25—C26—C27v	111.4 (4)v
C11—C10—C15v	118.6 (4)v	C25—C26—H26Av	109.3v
C11—C10—P2v	120.5 (3)v	C27—C26—H26Av	109.3v
C15—C10—P2v	120.9 (3)v	C25—C26—H26Bv	109.3v
C12—C11—C10v	120.3 (4)v	C27—C26—H26Bv	109.3v
C12—C11—H11v	119.8v	H26A—C26—H26Bv	108.0v
C10—C11—H11v	119.8v	C22—C27—C26v	110.4 (3)v
C13—C12—C11v	119.6 (5)v	C22—C27—H27Av	109.6v
C13—C12—H12v	120.2v	C26—C27—H27Av	109.6v
C11—C12—H12v	120.2v	C22—C27—H27Bv	109.6v
C14—C13—C12v	120.7 (4)v	C26—C27—H27Bv	109.6v
C14—C13—H13v	119.7v	H27A—C27—H27Bv	108.1v

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—Hv	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O6^{iv}	0.76 (4)v	1.88 (4)v	2.642 (4)v	178 (7)v
O5—H5A···O6^{iiv}	0.94 (7)v	1.67 (7)v	2.596 (4)v	169 (6)v
N—H10A···O3v	0.89 (2)v	1.92 (2)v	2.798 (4)v	169 (4)v
N—H10B···O3^{iiiv}	0.95 (4)v	1.83 (4)v	2.759 (4)v	165 (4)v

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, −*y*+1, −*z*+1; (iii) −*x*+2, −*y*+2, −*z*+1.v

Fig. 1m

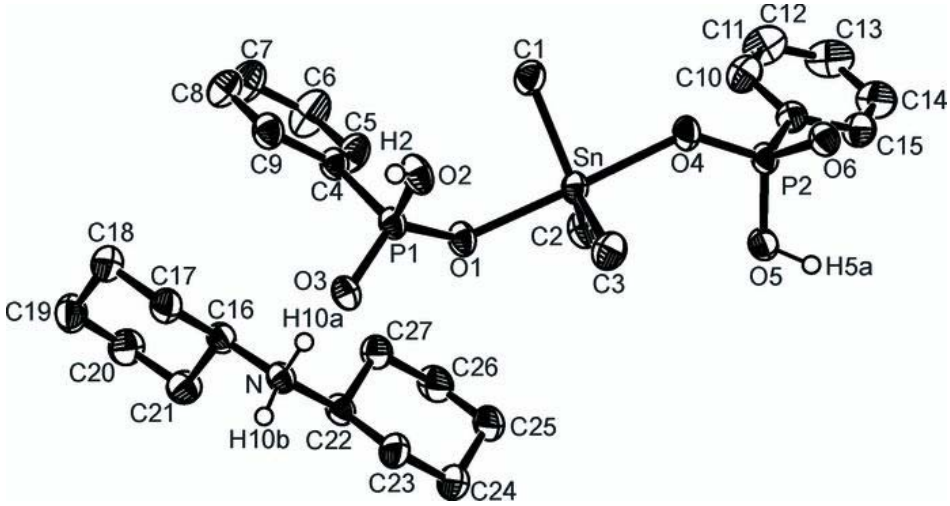

Fig. 2m